

B.I.A.G.R.A.

Bibliotec**A** de pro**G**Ramación científic**A**

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Contents

I	Introduction	7
1	What is <i>B.I.A.G.R.A</i> ?	9
1.1	C language?	9
1.2	Some general ideas about <i>B.I.A.G.R.A</i>	10
1.3	Como instalar <i>B.I.A.G.R.A</i> en LINUX	10
1.3.1	Intalación de la biblioteca <i>B.I.A.G.R.A</i> estática	10
II	<i>B.I.A.G.R.A</i> Data structures and constants	13
2	<i>B.I.A.G.R.A</i> constants (constants.h)	15
2.1	Introduction	15
2.2	Mathematical constants	15
2.3	Logical constants	15
2.4	Error constants	16
III	Memory allocation	17
3	Memory allocation (resmem.h)	19
3.1	Introduction	19
3.2	Vector's memory allocation	19
3.2.1	intPtMemAllocVec function	19
3.2.2	dblPtMemAllocVec function	19
3.3	Matrix memory allocation	20
3.3.1	dblPtMemAllocMat function	20
3.3.2	dblPtMemAllocUpperTrMat function	20
3.3.3	dblPtMemAllocLowerTrMat function	21
3.4	Freeing memory	22
3.4.1	freeMemDblMat function	22

IV	Mathematical functions	23
4	Pseudo random numbers (random.h)	25
4.1	Introduction	25
4.2	Pseudo random integer numbers	25
4.2.1	intRandom function	25
4.2.2	uintRandom function	26
4.3	Pseudo random floating point numbers	26
4.3.1	dblRandom function	26
4.3.2	udblRandom function	27
5	Complex numbers (complejo.h)	29
5.1	Introduction	29
5.2	Data structures	29
5.2.1	biaComplex data structure	29
5.2.2	biaPolar data structure	29
5.3	Arithmetical operations using complex numbers	30
5.3.1	addComplex function	30
5.3.2	subtractComplex function	31
5.3.3	multiplyComplex function	31
5.3.4	divideComplex function	32
5.3.5	invSumComplex function	32
5.3.6	invMulComplex function	33
5.4	Complex number operations	33
5.4.1	dblComplexModulus function	33
5.4.2	dblComplexArg function	33
5.4.3	conjugateComplex function	34
5.4.4	complex2Polar function	34
5.4.5	polar2Complex function	34
6	Integer numbers (integers.h)	35
6.1	Introduction	35
6.2	Sum integers	35
6.2.1	uintSumFirstNIntegers function	35
6.3	Prime numbers	35
6.3.1	isPrime function	35
6.3.2	getFirstNPrimes function	36
7	Polynomial (polynomials.h)	37
7.1	Introduction	37
7.2	Data structures	37

7.2.1	<code>biaRealPol</code> data structure	37
7.3	Polynomial derivatives	38
7.3.1	<code>derivativePol</code> function	38
7.4	Arithmetical operations using polynomials	39
7.4.1	<code>addPol</code> function	39
7.4.2	<code>subtractPol</code> function	40
7.4.3	<code>multiplyPol</code> function	40
8	Matrix (<code>matrix.h</code>)	43
8.1	Introduction	43
8.2	Data structures	43
8.2.1	<code>biaMatrix</code> data structure	43
8.3	Matrix creation	44
8.3.1	<code>identityMatrix</code> function	44
8.3.2	<code>scalingMatrix</code> function	45
8.3.3	<code>nullMatrix</code> function	45
8.4	Matrix operations	46
8.4.1	<code>transposeMatrix</code> function	46
8.5	Matrix checks	46
8.5.1	<code>isIdentityMatrix</code> function	46
8.5.2	<code>isNullMatrix</code> function	47
8.5.3	<code>isSymmetricMatrix</code> function	47
9	Roots approximation (<code>roots.h</code>)	49
9.1	Introduction	49
9.2	Data structures	49
9.2.1	<code>biaRealRoot</code> data structure	49
9.3	Function roots approximation	50
9.3.1	<code>newtonPol</code> function	50
9.3.2	<code>newtonMethod</code> function	51
10	Runge-Kutta methods (<code>rngkutta.h</code>)	53
10.1	Introduction	53
10.2	Data structures	53
10.2.1	<code>biaButcherArray</code> data structure	53
10.2.2	<code>biaDataRK</code> data structure	54
10.3	Node number calculations	55
10.3.1	<code>intNodeNumber</code> function	55
10.4	Explicit Runge-Kutta methods (scalar problems)	56
10.4.1	<code>ExplicitRungeKutta</code> function	56
10.4.2	<code>classicRungeKuttaCoefs</code> function	57

10.4.3	<code>heunRungeKuttaCoefs</code> function	58
10.4.4	<code>kuttaRungeKuttaCoefs</code> function	58
10.4.5	<code>modifiedEulerRungeKuttaCoefs</code> function	59
10.4.6	<code>improvedEulerRungeKuttaCoefs</code> function	60
A	Runge-Kutta methods	61
A.1	What is a Runge-Kutta method?	61
A.1.1	What is a I.V.P.?	61
A.2	Runge-Kutta's method notation	62
A.2.1	General formulation	62
A.2.2	Matricial notation (Butcher's)	62
A.3	Runge-Kutta types	63
A.3.1	Implicit Runge-Kutta	63
A.3.2	Semi-implicit Runge-Kutta	63
A.3.3	Explicit Runge-Kutta	63

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Part I
Introduction

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Chapter 1

What is *B.I.A.G.R.A* ?

- *B.I.A.G.R.A* stands for **B**ibliotec**A** de pro**G**ramación científic**A** which means Scientific Programming Library.
- *B.I.A.G.R.A* is entirely coded using **C** language.
- *B.I.A.G.R.A* has been developed and tested under *LINUX*.
- *B.I.A.G.R.A* is distributed as open source and its author does not take any responsibility.
- I wrote *B.I.A.G.R.A* in the 90s to help me with some academic tasks when studying my degree.

1.1 C language?

C language instead of **FORTRAN**?

- **C** is modular and structured.
- **C** is a general purpose language programming.
- **C** is a very powerful language and its code is very fast.
- **C** allows dynamic memory allocation.
- **C** code is portable.
- **C** is able to handle graphic modes.

1.2 Some general ideas about *B.I.A.G.R.A*

B.I.A.G.R.A has been developed under **Linux** and some **Linux** knowledge is needed.

B.I.A.G.R.A was developed to solve general problems instead of particular ones. For instance, instead of writing a program to get the inverse of a 4x4 matrix and having to change the source code to get the inverse of a 5x5 matrix *B.I.A.G.R.A* was developed to allow to write programs to get the inverse of any matrix without having to change de sorce code.

To be able to do that *pointers* were used instead of using *arrays*.

When we talk about *vectors* we will be talking about a *pointer* using dynamic memory allocation. When we talk about matrices we will be talking about *pointer* to a *pointer* using dynamic memory allocation.

B.I.A.G.R.A uses some data structures to store data.

For common errors as:

- Errors in dynamic memory allocation.
- Division by zero.
- ...

B.I.A.G.R.A uses its own constants to notify these errors (Chapter 2).

1.3 Como instalar *B.I.A.G.R.A* en LiNux

Para instalar *B.I.A.G.R.A* lo primero que hay que hacer es entrar en el sistema como **root** y situarse en el directorio donde esten los fuentes de la biblioteca.

1.3.1 Intalación de la biblioteca *B.I.A.G.R.A* estática

Para instalar este tipo bibilioteca se puede hacer de dos formas:

1. *./instalar estatica*

2. *make estatica*

En realidad ambas hacen lo mismo, la opción con *make* en realidad ejecuta *./instalar estatica*.

Al realizar cualquiera de estas dos opciones se copiarán los ficheros cabecera a ***/usr/include/biagra*** y a continuación se creará la biblioteca ***/usr/lib/libbiagra.a***.

Luego si se utiliza una función de esta biblioteca, cuyo prototipo está en el fichero de cabecera *rngkutta.h* habrá que incluir en las directivas al preprocesador **`#include <biagra/rngkutta.h>`**.

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Part II

B.I.A.G.R.A Data structures
and constants

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Chapter 2

B.I.A.G.R.A constants (const.h)

2.1 Introduction

B.I.A.G.R.A includes its own constants to be used if needed.

These constants are defined in `const.h`.

2.2 Mathematical constants

Table 2.1 shows the *B.I.A.G.R.A* 's mathematical constants.

Constant	Name	Value
e	BIA_E	2.71828182845904523536029
π	BIA_PI	3.14159265358979323846264

Table 2.1: *B.I.A.G.R.A* mathematical constants.

2.3 Logical constants

The following logical constants are defined:

BIA_FALSE when a condition is not met.

BIA_TRUE when a condition is met.

2.4 Error constants

The following error constants are defined:

BIA_ZERO_DIV division by zero.

BIA_MEM_ALLOC error in memory allocation.

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Part III

Memory allocation

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Chapter 3

Memory allocation (resmem.h)

3.1 Introduction

B.I.A.G.R.A includes its own memory allocation functions which are defined in `resmem.h` file.

3.2 Vector's memory allocation

Some functions are provided to handle memory allocations for vectors.

3.2.1 `intPtMemAllocVec` function

This functions allocates memory for a vector of `int`.

The definition of this function:

```
double *intPtMemAllocVec(int intElements);
```

This function has only one argument, `intElements`, which is the dimension of the vector and a `int` pointer is returned.

3.2.2 `dblPtMemAllocVec` function

This functions allocates memory for a vector of doubles.

The definition of this function:

```
double *dblPtMemAllocVec(int intElements);
```

This function has only one argument, `intElements`, which is the dimension of the vector and a `double` pointer is returned.

3.3 Matrix memory allocation

Some functions are provided to handle memory allocations for vectors.

3.3.1 dblPtMemAllocMat function

This function allocates memory for a matrix of doubles.

The definition of this function:

```
double **dblPtMemAllocMat(int intRows, int intCols);
```

where:

intRows number of rows.

intCols number of columns.

3.3.2 dblPtMemAllocUpperTrMat function

This function allocates memory for a upper triangular square matrix.

The definition of this function:

```
double **dblPtMemAllocUpperTrMat(int intOrder);
```

This function has only one argument, **intOrder**, which is the order of the matrix and a **double** pointer to pointer is returned.

In a upper triangular square matrix all elements below the diagonal are zero:

$$\begin{pmatrix} a_{0,0} & a_{0,1} & a_{0,2} & a_{0,3} & a_{0,4} \\ 0 & a_{1,1} & a_{1,2} & a_{1,3} & a_{1,4} \\ 0 & 0 & a_{2,2} & a_{2,3} & a_{2,4} \\ 0 & 0 & 0 & a_{3,3} & a_{3,4} \\ 0 & 0 & 0 & 0 & a_{4,4} \end{pmatrix}$$

For **intOrder** = 5:

```
myMatrix = dblPtMemAllocUpperTrMat(5);
```

and:

B.I.A.G.R.A

Pointer	# elements	First element	Last element
myMatrix[0]	5	0	4
myMatrix[1]	4	0	3
myMatrix[2]	3	0	2
myMatrix[3]	2	0	1
myMatrix[4]	1	0	0

so:

$$myMatrix[i][j] = (*(myMatrix + i) + j) = \begin{cases} a_{i,j+i} & \forall i \leq j \\ 0 & \forall i > j \end{cases}$$

3.3.3 dblPtMemAllocLowerTrMat function

This function allocates memory for a lower triangular square matrix.

The definition of this function:

```
double **dblPtMemAllocLowerTrMat(int intOrder);
```

This function has only one argument, `intOrder`, which is the order of the matrix and a double pointer to pointer is returned.

In a lower triangular square matrix all elements above the diagonal are zero:

$$\begin{pmatrix} a_{0,0} & 0 & 0 & 0 & 0 \\ a_{1,0} & a_{1,1} & 0 & 0 & 0 \\ a_{2,0} & a_{2,1} & a_{2,2} & 0 & 0 \\ a_{3,0} & a_{3,1} & a_{3,2} & a_{3,3} & 0 \\ a_{4,0} & a_{4,1} & a_{4,2} & a_{4,3} & a_{4,4} \end{pmatrix}$$

For `intOrder = 5`:

```
myMatrix = dblPtMemAllocLowerTrMat(5);
```

and:

Pointer	# elements	First element	Last element
myMatrix[0]	1	0	0
myMatrix[1]	2	0	1
myMatrix[2]	3	0	2
myMatrix[3]	4	0	3
myMatrix[4]	5	0	4

so:

$$myMatrix[i][j] = *((*(myMatrix + i) + j)) = \begin{cases} a_{i,j} & \forall i \leq j \\ 0 & \forall i < j \end{cases}$$

3.4 Freeing memory

B.I.A.G.R.A includes its own functions to free memory.

3.4.1 freeMemDblMat function

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Part IV
Mathematical functions

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Chapter 4

Pseudo random numbers (random.h)

4.1 Introduction

B.I.A.G.R.A includes its own functions to pseudo random number generation and they are defined in `random.h` file.



This functions have not been tested to produce unpredictable sequences, so be careful when use them.

4.2 Pseudo random integer numbers

4.2.1 `intRandom` function

This function generates random integers.

The definition of this function:

```
int intRandom(int limit);
```

The pseudo random integer is placed in the interval $(-limit, limit)$.



*Before using this function **srand** must be used to initialize **rand**. You can use `srand((unsigned)time(NULL))`.*

The pseudo random number is generated with the following formula:

$$\left[\frac{\text{limit} \cdot \text{rand}()}{\text{RAND_MAX} + 1} \right] \in (-\text{limit}, \text{limit})$$

Then randomly is choosed if the number is positive or negative using the above formula with $\text{limit} = 2$ and then taking modulus 2. If modulus is 1 then the number will be a negative one.

4.2.2 uintRandom function

This function generates random integers.

The definition of this function:

```
int uintRandom(int limit);
```

The pseudo random integer is placed in the interval $[0, \text{limit})$.



*Before using this function **srand** must be used to initialize **rand**. You can use **srand((unsigned)time(NULL))**.*

The pseudo random number is generated with the following formula:

$$\left[\frac{\text{limit} \cdot \text{rand}()}{\text{RAND_MAX} + 1} \right] \in [0, \text{limit})$$

4.3 Pseudo random floating point numbers

4.3.1 dblRandom function

This function generates random floating point numbers.

The definition of this function:

```
int dblRandom(int limit);
```

The pseudo random floating point number is placed in the interval $(-\text{limit}, \text{limit})$.



*Before using this function **srand** must be used to initialize **rand**. You can use **srand((unsigned)time(NULL))**.*

The pseudo random number is generated with the following formula:

$$\frac{\text{limit} \cdot \text{rand}()}{\text{RAND_MAX} + 1} \in (-\text{limit}, \text{limit})$$

Then randomly is choosed if the number is positive or negative using the above formula with $\text{limit} = 2$ and then taking modulus 2. If modulus is 1 then the number will be a negative one.

4.3.2 udblRandom function

This function generates random floating point numbers.

The definition of this function:

```
int udblRandom(int limit);
```

The pseudo random floating point number is placed in the interval $[0, \text{limit})$.



*Before using this function **rand** must be used to initialize **rand**. You can use **srand((unsigned)time(NULL))**.*

The pseudo random number is generated with the following formula:

$$\frac{\text{limit} \cdot \text{rand}()}{\text{RAND_MAX} + 1} \in [0, \text{limit})$$

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Chapter 5

Complex numbers (complejo.h)

5.1 Introduction

Functions to manage complex numbers are defined in `complex.h` file.

5.2 Data structures

Some data structures are defined in *B.I.A.G.R.A.* to manage complex numbers.

5.2.1 `biaComplex` data structure

This data structure is used to handle polynomials $p(x) \in \mathbb{R}[x]$. `biaComplex` data structure is defined in figure 7.1 where:

intDegree polynomial degree.

intRealRoots number of real roots (if any).

intCompRoots number of complex roots (if any).

***dblCoef** pointer to store polynomial coefficients.

5.2.2 `biaPolar` data structure

This data structure is used to store data for root approximation. Data structure is defined in figure 9.1 where:

```
typedef struct {  
    double dblReal,  
           dblImag;  
} biaComplex;
```

Figure 5.1: biaComplex data structure.

intNMI maximum number of iterations to get the root with a maximum error of *dblTol*.

intIte iterations used to get the root.

dblx0 initial approximation to get the root.

dblRoot root approximation.

dblTol maximum tolerance when calculating the root.

dblError error in root approximation. Difference between the last two root approximations.

```
typedef struct {  
    double dblMod,  
           dblArg;  
} biaPolar;
```

Figure 5.2: biaPolar data structure.

5.3 Arithmetical operations using complex numbers

5.3.1 addComplex function

This function adds two complex numbers.

The definition of this function:

```
void addComplex(biaComplex *ptCmplx1, biaComplex *ptCmplx2,  
               biaComplex *ptRes);
```

where:

***ptCmplx1** first complex number to be added.

***ptCmplx2** second complex number to be added.

***ptRes** result of the operation.

5.3.2 subtractComplex function

This function subtracts two complex numbers.

The definition of this function:

```
void subtractComplex(biaComplex *ptCmplx1, biaComplex *ptCmplx2,  
                    biaComplex *ptRes);
```

where:

***ptCmplx1** complex number.

***ptCmplx2** complex number to be subtracted to the above.

***ptRes** result of the operation.

5.3.3 multiplyComplex function

This function multiplies two complex numbers.

The definition of this function:

```
void multiplyComplex(biaComplex *ptCmplx1, biaComplex *ptCmplx2,  
                    biaComplex *ptRes);
```

where:

ptCmplx1 first complex number to be multiplied.

ptCmplx2 second complex number to be multiplied.

ptRes result of the operation.

5.3.4 divideComplex function

This function divides one complex number by other:

$$\frac{a + b \cdot i}{c + d \cdot i} = (a + b \cdot i) \cdot (c + d \cdot i)^{-1}$$

The definition of this function:

```
int divideComplex(biaComplex *ptCmplx1, biaComplex *ptCmplx2,
                 biaComplex *ptRes);
```

where:

***ptCmplx1** complex number.

***ptCmplx2** complex number used as divisor.

***ptRes** result of the operation.

The following codes are returned:

BIA_ZERO_DIV	Division by zero
BIA_TRUE	Success

5.3.5 invSumComplex function

This function gets the additive inverse of a complex number:

$$\forall z_1 \in \mathbb{C} \quad \exists z_2 \in \mathbb{C} \mid z_1 + z_2 = 0$$

The definition of this function:

```
void invSumComplex(biaComplex *ptCmplx, biaComplex *ptRes);
```

where:

***ptCmplx** complex number to get its additive inverse.

***ptRes** where the additive inverse will be stored.

5.3.6 invMulComplex function

This function gets the multiplicative inverse of a complex number:

$$\forall z_1 \in \mathbb{C} - \{0\} = \mathbb{C}^* \quad \exists z_2 \in \mathbb{C} \mid z_1 \cdot z_2 = 1$$

The definition of this function:

```
int invMulComplex(biaComplex *ptCmplx, biaComplex *ptRes) ;
```

where:

***ptCmplx** complex number to get its multiplicative inverse.

***ptRes** where the additive multiplicative will be stored.

The following codes are returned:

BIA_ZERO_DIV	Division by zero
BIA_TRUE	Success

5.4 Complex number operations

5.4.1 dblComplexModulus function

This function gets the modulus of a complex number.

The definition of this function:

```
double dblComplexModule(biaComplex *ptCmplx);
```

where:

***ptCmplx** complex number to get its modulus.

This function returns the complex number modulus.

5.4.2 dblComplexArg function

This function gets the argument of a complex number.

The definition of this function:

```
double dblComplexArg(biaComplex *ptCmplx);
```

where:

***ptCmplx** complex number to get its argument.

This function returns the complex number argument (radians).

5.4.3 conjugateComplex function

This function gets the conjugate complex of a complex number:

$$z = a + b \cdot i \in \mathbb{C} \Rightarrow \bar{z} = a - b \cdot i \in \mathbb{C}$$

The definition of this function:

```
void conjugateComplex(biaComplex *ptCmplx, biaComplex *ptRes);
```

where:

***ptCmplx** complex number to get its conjugate.

***ptRes** complex conjugate.

5.4.4 complex2Polar function

This function gets the polar coordinates of a complex number.

The definition of this function:

```
void complex2Polar(biaComplex *ptCmplx, biaPolar *ptRes);
```

where:

***ptCmplx** complex number to calculate polar coordinates.

***ptRes** polar coordinates.

5.4.5 polar2Complex function

This function gets the cartesian coordinates of a polar coordinates for a complex number.

The definition of this function:

```
void polar2Complex(biaPolar *ptPolar, biaComplex *ptRes);
```

where:

***ptPolar** polar coordinates.

***ptRes** complex number in cartesian coordinates.



Argument is supposed to be in radians.

Chapter 6

Integer numbers (integers.h)

6.1 Introduction

B.I.A.G.R.A includes functions about integer numbers in `integers.h` file.

6.2 Sum integers

6.2.1 `uintSumFirstNIntegers` function

This function gets the sum of the first n integers.

The definition of this function:

```
unsigned uintSumFirstNIntegers(int n);
```

If the sum is bigger than an unsigned int 0 is returned.

6.3 Prime numbers

6.3.1 `isPrime` function

This function checks if a number is a prime number.

The definition of this function:

```
int isPrime(int intN);
```

The following codes are returned:

BIA_FALSE	intN is not a prime number
BIA_TRUE	intN is a prime number

6.3.2 `getFirstNPrimes` function

This function checks if a number is a prime number.

The definition of this function:

```
void getFirstNPrimes(unsigned int *ptPrimes, int intNumber, int *ptCalc);
```

where:

***ptPrimes** array where primes will be stored. Memory allocation for this array has to be initialized before using this function.

intNumber number of primes to be computed.

***ptCalc** in this variable the total amount of computed primes will be stored.

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Chapter 7

Polynomial (polynomials.h)

7.1 Introduction

Functions to manage polynomials are defined in `polynomial.h` file.

A polynomial used to be represented as shown in equation 7.1.

$$p(x) = a_0 + a_1 \cdot x + \cdots + a_n \cdot x^n = \sum_{i=0}^n a_i \cdot x^i \quad \text{where } a_i \in \mathbb{R} \quad (7.1)$$

7.2 Data structures

Some data structures are defined in *B.I.A.G.R.A* to manage polynomials.

7.2.1 `biaRealPol` data structure

This data structure is used to handle polynomials $p(x) \in \mathbb{R}[x]$. **biaPol** data structure is defined in figure 7.1 where:

intDegree polynomial degree.

intRealRoots number of real roots (if any).

intCompRoots number of complex roots (if any).

***dblCoef** pointer to store polynomial coefficients.

```
typedef struct {
    int  intDegree    = 0,
        intRealRoots = 0,
        intCompRoots = 0;

    double *dblCoefs;
} biaRealPol;
```

Figure 7.1: biaRealPol data structure.

Polynomial coefficients are stored in `dblCoefs` pointer which has to be previously initialized:

```
dblCoefs[0] = a0
dblCoefs[1] = a1
...
dblCoefs[n] = an
```

7.3 Polynomial derivatives

7.3.1 derivativePol function

This function gets the n -th derivative of a polynomial.

The definition of this function:

```
int derivativePol(biaPol *ptPol, biaPol *ptDer, int intN);
```

where:

***ptPol** pointer to a `biaRealPol` struct with the polynomial to get its derivative is stored.

***ptDer** pointer to a `biaRealPol` struct where the derivative will be stored.

intN order of the derivative to get.

The following codes are returned:

BIA_MEM_ALLOC	Memory allocation error
BIA_TRUE	Success



***ptDer** will be released and memory allocation will be carried out to store the derivative.*



***ptDer** member **dblCoefs** has to be initialized to a **NULL** pointer to avoid a **Segment Fault** error if it was not previously initialized.*

7.4 Arithmetical operations using polynomials

7.4.1 addPol function

This function adds two polynomials.

The definition of this function:

```
int addPol(biaPol *ptPol1, biaPol *ptPol2, biaPol *ptRes);
```

where:

***ptPol1** pointer to a **biaPol** struct with the first polynomial to be added.

***ptPol2** pointer to a **biaPol** struct with the second polynomial to be added.

***ptRes** pointer to a **biaPol** struct where the add operation will be stored.

The following codes are returned:

BIA_MEM_ALLOC	Memory allocation error
BIA_TRUE	Success



***ptRes** will be released and memory allocation will be carried out to store the derivative.*



***ptRes** member **dblCoefs** has to be initialized to a **NULL** pointer to avoid a **Segment Fault** error if it was not previously initialized.*

7.4.2 subtractPol function

This function subtracts two polynomials.

The definition of this function:

```
int subtractPol(biaPol *ptPol1, biaPol *ptPol2, biaPol *ptRes);
```

where:

***ptPol1** pointer to a `biaPol` struct with the first polynomial.

***ptPol2** pointer to a `biaPol` struct with the polynomial to be subtracted from the above.

***ptRes** pointer to a `biaPol` struct where the subtract operation will be stored.

The following codes are returned:

BIA_MEM_ALLOC	Memory allocation error
BIA_TRUE	Success



***ptRes** will be released and memory allocation will be carried out to store the derivative.*

***ptRes** member **dblCoefs** has to be initialized to a **NULL** pointer to avoid a **Segment Fault** error if it was not previously initialized.*

7.4.3 multiplyPol function

This functions multiplies two polynomials.

The definition of this function:

```
int subtractPol(biaPol *ptPol1, biaPol *ptPol2, biaPol *ptRes);
```

where:

***ptPol1** pointer to a `biaPol` struct with the first polynomial.

***ptPol2** pointer to a `biaPol` struct with the second polynomial.

***ptRes** pointer to a **biaPol** struct where the multiplication operation will be stored.

The following codes are returned:

BIA_MEM_ALLOC	Memory allocation error
BIA_TRUE	Success



ptRes will be released and memory allocation will be carried out to store the derivative.



ptRes member *dblCoefs* has to be initialized to a *NULL* pointer to avoid a **Segment Fault** error if it was not previously initialized.

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Chapter 8

Matrix (matrix.h)

8.1 Introduction

Functions to manage matrices are defined in `matrix.h` file.

8.2 Data structures

Some data structures are defined in *B.L.A.G.R.A* to manage matrices.

8.2.1 `biaMatrix` data structure

This data structure is used to store a matrix. `biaMatrix` data structure is defined in figure 8.1 where:

`intRows` number of rows.

`intCols` number of columns.

`**dblCoefs` pointer to store matrix coefficients.

```
typedef struct {
    int intRows,
        intCols;

    double **dblCoefs;
} biaMatrix;
```

Figure 8.1: biaMatrix data structure.

8.3 Matrix creation

B.I.A.G.R.A includes functions to create some kind of matrices.

8.3.1 identityMatrix function

This function stores the identity matrix with order taken from `intRows` member of `ptMatrix`:

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & \ddots & 0 & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & \ddots & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

The definition of this function:

```
void identityMatrix(biaMatrix *ptMatrix);
```

where:

***ptMatrix** matrix that has to be created before using this function. Memory allocation for `dblCoefs` must be done before using this function.



intRows is used to get the matrix order.

8.3.2 scalingMatrix function

This function stores the scaling matrix with factor λ and order taken from `intRows` member of `ptMatrix`:

$$\begin{pmatrix} \lambda & 0 & 0 & 0 & 0 \\ 0 & \lambda & \ddots & 0 & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & \ddots & \lambda & 0 \\ 0 & 0 & 0 & 0 & \lambda \end{pmatrix}$$

The definition of this function:

```
void scalingMatrix(biaMatrix *ptMatrix, double dblFactor);
```

where:

***ptMatrix** matrix that has to be created before using this function. Memory allocation for `dblCoefs` must be done before using this function.



intRows is used to get the matrix order.

8.3.3 nullMatrix function

This function stores the null matrix with order taken from `intRows` member of `ptMatrix`:

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \ddots & 0 & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & \ddots & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

The definition of this function:

```
void nullMatrix(biaMatrix *ptMatrix);
```

where:

***ptMatrix** matrix that has to be created before using this function. Memory allocation for `dblCoefs` must be done before using this function.



intRows and intCols is used to get the matrix order.

8.4 Matrix operations

8.4.1 transposeMatrix function

This function stores the transpose matrix of a given matrix.

The definition of this function:

```
void transposeMatrix(biaMatrix *ptMatrix, biaMatrix *ptRes);
```

where:

***ptMatrix** matrix to get its transpose matrix.

***ptRes** matrix to store the transpose matrix. Memory has to be preallocated before using this function.



intRows and intCols is used to get the matrix order.

8.5 Matrix checks

8.5.1 isIdentityMatrix function

This function checks if a matrix is the identity matrix.

The definition of this function:

```
int isIdentityMatrix(biaMatrix *ptMatrix);
```

where:

***ptMatrix** matrix to check.

8.5.2 isNullMatrix function

This function checks if a matrix is a null matrix.

The definition of this function:

```
int isNullMatrix(biaMatrix *ptMatrix, double dblTol);
```

where:

***ptMatrix** matrix to check.

dblTol if a matrix element is minor than this value it is assumed it is a null element.

8.5.3 isSymmetricMatrix function

This function checks if a matrix is a symmetric matrix.

The definition of this function:

```
int isSymmetricMatrix(biaMatrix *ptMatrix);
```

where:

***ptMatrix** matrix to check.

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Chapter 9

Roots approximation (roots.h)

9.1 Introduction

Functions to compute function's roots approximation are defined in `roots.h` file.

9.2 Data structures

Some data structures are defined in *B.L.A.G.R.A* to manage roots.

9.2.1 `biaRealRoot` data structure

This data structure is used to store data for root approximation.

Data structure is defined in figure 9.1 where:

intNMI maximum number of iterations to get the root with a maximum error of `dblTol`.

intIte iterations used to get the root.

dblX0 initial approximation to get the root.

dblRoot root approximation.

dblTol maximum tolerance when calculating the root.

dblError error in root approximation. Difference between the last two root approximations.

```
typedef struct {
    int intMNI,
        intIte;

    double dblx0,
        dblRoot,
        dblTol,
        dblError;
} biaRealRoot;
```

Figure 9.1: biaRealRoot data structure.

9.3 Function roots approximation

9.3.1 newtonPol function

This function approaches a polynomial root using the **Newton** method.

The definition of this function:

```
int newtonPol(biaPol *ptPol, biaRealRoot *ptRoot);
```

The following codes are returned:

BIA_MEM_ALLOC	Memory allocation error
BIA_ZERO_DIV	Division by zero
BIA_TRUE	the root was computed satisfying the problem conditions (intMNI and dblTol);
BIA_FALSE	Root approximation could not be calculated satisfying the requirements (intMNI and dblTol).

The following values in ***ptRoot** need to be initialized:

intMNI maximun number of iterations to compute the root.

dblx0 initial approximation.

dblTol tolerance to compute de root.

The following data will be stored:

intIte iterations used to compute the root.

dblRoot approximation of the root.

dblError error in the approximation.



*When two consecutive approximations are close enough, **dblTol**, last approximation will be considered as good and will be stored in ***biaRealRoot** ***ptRoot** in **dblRoot**.*

9.3.2 newtonMethod function

This function approaches a function's root using the **Newton** method.

The definition of this function:

```
int newtonMethod(biaRealRoot *ptRoot,
                int (*func)(double dblx0, double *ptRes),
                int (*der)(double dblx0, double *ptRes));
```

Function's pointers are used to avoid having to recode the C function every time a root function need to be approximated for different mathematical functions.

The following codes are returned:

BIA_ZERO_DIV	Division by zero
BIA_TRUE	the root was computed satisfying the problem conditions (intMNI and dblTol);
BIA_FALSE	Root approximation could not be calculated satisfying the requirements (intMNI and dblTol).

where:

***ptRoot** is a pointer to a **biaRealRoot** variable.

***func** pointer to a function implementing the function which root is going to be computed.

***der** pointer to a function implementing the derivative of the function which root is going to be computed.

The following values in ***ptRoot** need to be initialized:

intMNI maximum number of iterations to compute the root.

dblx0 initial approximation.

dblTol tolerance to compute de root.

The following data is stored:

intIt iterations used to compute the root.

dblRoot approximation of the root.

dblError error in the approximation.



*When two consecutive approximations are close enough, **dblTol**, last approximation will be considered as good and will be stored in ***biaRealRoot** ***ptRoot** in **dblRoot**.*

Usage example

To approximate a root for the function $f(x) = \sqrt{2}$ to C functions need to be created. A C function for the mathematical function implementation:

```
/* f(x) = x^2 - 2 */
int myfunc(double x0, double *fx0) {
    *fx0 = (double)(x0 * x0 - 2.);
    return BIA_TRUE;
}
```

A C function for the mathematical derivative function implementation:

```
/* f'(x) = 2*x */
int myfuncder(double x0, double *fx0) {
    *fx0 = 2.*x0;
    return BIA_TRUE;
}
```

Both functions must meet the following requirements:

- An integer value is returned, **BIA_TRUE** when function is evaluated in $x0$ and **BIA_ZERO_DIV** if a division by zero takes place.
- $x0$ value to evaluate the function.
- $*fx0$ pointer to a double to store the function's value in $x0$.

So to approximate function's root using Newton Method:

```
i = newtonMethod(&myRoot, &myfunc, &myfuncder);
```

Chapter 10

Runge-Kutta methods (rngkutta.h)

10.1 Introduction

Runge-Kutta are a family of implicit and explicit iterative methods used to approximate solutions of ordinary differential equations or **ODE**.

Butcher matricial notation is used in this implementation.

10.2 Data structures

10.2.1 `biaButcherArray` data structure

This structure is used to store the Butcher matricial notation.

Data structure is defined in figure [10.1](#) where:

intStages method stages.

***dblC** c_i coefficients stored in an array with size **intStages**.

***dblB** b_i coefficients stored in an array with size **intStages**.

****dblMatrix** matrix to store $a_{i,j}$ method's coefficients.

```
typedef struct {
    double  *dblC,
            *dblB,
            **dblMatrix;

    int      intStages;
} biaButcherArray;
```

Figure 10.1: biaButcherArray data structure.



See appendix A if you need information about Butcher matrix notation.

10.2.2 biaDataRK data structure

This structure is used to store all the data needed to apply a Runge-Kutta method.

Data structure is defined in figure 10.2 where:

intNumApprox number of approximations to be done (size of the array `dblPoints`).

intImplicit when the Runge-Kutta method is implicit or not. The following constants are defined in the header file:

Name	Value
BIA_IMPLICIT_RK_TRUE	0
BIA_IMPLICIT_RK_FALSE	1

***dblPoints** array with dimension `intNumApprox` and its elements will be the approximations in x_i where:

$$x_i = dblFirst + i \cdot dblStepSize \quad \text{where} \quad 0 \leq i < intNumApprox$$

dblStepSize method's step-size.

dblFirst first point used to compute all the approximations. The value of the function in this point is known (initial condition).

dblLast last point in which approximations will be computed.

strCoefs variable of type `biaButcherArray` (section 10.2.1) storing Butcher matricial notation.

```
typedef struct {  
    int intNumApprox,  
        intImplicit;  
  
    double *dblPoints,  
        dblStepSize,  
        dblFirst,  
        dblLast;  
  
    biaButcherArray strCoefs;  
} biaDataRK;
```

Figure 10.2: `biaDataRK` data structure.

10.3 Node number calculations

10.3.1 `intNodeNumber` function

This function gets the number of nodes that can be placed in an interval. All nodes are equidistant.

The definition of this function:

```
int intNodeNumber(double dblLong, double dblStepSize)
```

where:

dblLong interval length.

dblStepSize distance between two nodes.

The function returns the number of nodes that can be placed.



Arguments are supposed to be different from zero.



Arguments are supposed to be positive.

10.4 Explicit Runge-Kutta methods (scalar problems)

10.4.1 ExplicitRungeKutta function

This function solves an *I.V.P.* using an explicit Runge-Kutta method.

The definition of this function:

```
int explicitRungeKutta(biaDataRK *ptData,
                      double (*IVP)(double dblX, double dblY)
```

where:

ptData pointer to a **biaDataRK** variable¹. This variable contains all the necessary data to solve the *I.V.P.*

PVI C function's pointer to a function implementing the *O.D.E.*. This function needs to have two double arguments and returns the value of the *I.V.P.*:

dblX point where we want to evaluate the *O.D.E.*

dblY *O.D.E.* value in **dblX** ($y_i \approx y(x_i)$).

The following codes are returned:

BIA_MEM_ALLOC	Memory error allocation
BIA_TRUE	Success

Usage example

For instance, to solve this *I.V.P.*:

$$\begin{cases} y' = y(x) * \frac{x-y(x)}{x^2} \\ y(1) = 2 \end{cases}$$

the implementation of the IVP would be:

```
double IVP(double dblX, double dblY) {
    double  dblResultado;

    dblRes = dblY*((dblX-dblY)/(dblX*dblX));

    return (dblRes);
}
```

¹Section (10.2.2).

A **biaDataRK** variable has to be initialized. *B.I.A.G.R.A* provides several functions to initialize the **biaButcherArray** member.

To solve the *I.V.P.* problem:

```
i = explicitRungeKutta(&varDataRK, IVP);
```

10.4.2 classicRungeKuttaCoefs function

This function initialize the Butcher array for the classic Runge-Kutta method (four-stage method and order two).

The definition of this function:

```
int classicRungeKuttaCoefs(biaDataRK *ptData);
```

where:

ptData pointer to a **biaDataRK** variable². In this variable the following members will be initialized:

intStages will be initialized to 4.

intImplicit will be initialized to **BIA_IMPLICIT_RK_FALSE**.

strCoefs will be initialized with the Butcher array.

The Butcher array for this method:

$$\begin{array}{c|cccc} 0 & 0 & & & \\ \frac{1}{2} & \frac{1}{2} & 0 & & \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & \\ 1 & 0 & 0 & 1 & 0 \\ \hline & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \end{array}$$

The following codes are returned:

BIA_MEM_ALLOC	Memory error allocation
BIA_TRUE	Success

²Section (10.2.2).

10.4.3 heunRungeKuttaCoefs function

This function initialize the Butcher array for the Heun Runge-Kutta method (three-stage method and order three).

The definition of this function:

```
int heunRungeKuttaCoefs(biaDataRK *ptData);
```

where:

ptData pointer to a **biaDataRK** variable³. In this variable the following members will be initialized:

intStages will be initialized to 3.

intImplicit will be initialized to **BIA_IMPLICIT_RK_FALSE**.

strCoefs will be initialized with the Butcher array.

The Butcher array for this method:

0	0	0	0
1	$\frac{1}{3}$	0	0
2	0	$\frac{2}{3}$	0
3	$\frac{1}{4}$	0	$\frac{3}{4}$

The following codes are returned:

BIA_MEM_ALLOC	Memory error allocation
BIA_TRUE	Success

10.4.4 kuttaRungeKuttaCoefs function

This function initialize the Butcher array for the Kutta Runge-Kutta method (three-stage method and order three).

The definition of this function:

```
int kuttaRungeKuttaCoefs(biaDataRK *ptData);
```

where:

ptData pointer to a **biaDataRK** variable⁴. In this variable the following members will be initialized:

³Section (10.2.2).

⁴Section (10.2.2).

intStages will be initialized to 3.

intImplicit will be initialized to `BIA_IMPLICIT_RK_FALSE`.

strCoefs will be initialized with the Butcher array.

The Butcher array for this method:

$$\begin{array}{c|ccc} 0 & 0 & & \\ \frac{1}{2} & \frac{1}{2} & 0 & \\ 1 & -1 & 2 & 0 \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array}$$

The following codes are returned:

BIA_MEM_ALLOC	Memory error allocation
BIA_TRUE	Success

10.4.5 modifiedEulerRungeKuttaCoefs function

This function initialize the Butcher array for the modified Euler Kutta Runge-Kutta method (two-stage method and order two).

The definition of this function:

```
int modifiedEulerRungeKuttaCoefs(biaDataRK *ptData);
```

where:

ptData pointer to a **biaDataRK** variable⁵. In this variable the following members will be initialized:

intStages will be initialized to 2.

intImplicit will be initialized to `BIA_IMPLICIT_RK_FALSE`.

strCoefs will be initialized with the Butcher array.

The Butcher array for this method:

$$\begin{array}{c|cc} 0 & 0 & \\ \frac{1}{2} & \frac{1}{2} & 0 \\ \hline & 0 & 1 \end{array}$$

The following codes are returned:

BIA_MEM_ALLOC	Memory error allocation
BIA_TRUE	Success

⁵Section (10.2.2).

10.4.6 improvedEulerRungeKuttaCoefs function

This function initialize the Butcher array for the improved Euler Runge-Kutta method (two-stage method and order two).

The definition of this function:

```
int improvedRungeKuttaCoefs(biaDataRK *ptData);
```

where:

ptData pointer to a **biaDataRK** variable⁶. In this variable the following members will be initialized:

intStages will be initialized to 3.

intImplicit will be initialized to `BIA_IMPLICIT_RK_FALSE`.

strCoefs will be initialized with the Butcher array

The Butcher array for this method:

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

The following codes are returned:

BIA_MEM_ALLOC	Memory error allocation
BIA_TRUE	Success

⁶Section (10.2.2).

Appendix A

Runge-Kutta methods

This appendix is intended to help to know how Runge-Kutta methods are implemented and used in this library.

A.1 What is a Runge-Kutta method?

Runge-Kutta methods are a family of numerical methods to approach solutions of ordinary differential equations (O.D.E). These methods are iterative methods used to solve “*initial problem value*” (**I.P.V**) or “*Cauchy problem*”.

These methods are only-one-step methods with a fixed size for the method step¹.

A.1.1 What is a I.V.P.?

An *I.V.P.* is:

$$\begin{cases} y' = f(x, y(x)) \\ y(x_0) = y_0 \end{cases} \quad (\text{A.1})$$

So y' is a function depending on the variable x , and the function $y(x)$. $y(x)$ is the solution of the equation A.1 and the point (x_0, y_0) belongs to the curve $y(x)$.

Solving the *I.V.P.* A.1 is finding a function $y(x)$ such as the equation A.1 is met.

¹It is also possible to implement methods with a variable step known as *embedding*.

An example of a *I.V.P.*:

$$\begin{cases} y' = \frac{x*y(x)-y(x)^2}{x^2} \\ y(1) = 2 \end{cases} \quad (\text{A.2})$$

The solution of the A.2 will be:

$$y(x) = \frac{x}{\frac{1}{2} + \ln x} \quad (\text{A.3})$$

A.2 Runge-Kutta's method notation

$y(x_i)$ will be the exact value of the function $y(x)$ evaluated in x_i .

y_i will be the approximation of the function $y(x)$ in the point x_i .

h is the step used by the method in each iteration.

A.2.1 General formulation

A s -stages **Runge-Kutta's** method formulation is:

$$y_{n+1} = y_n + h \cdot \sum_{i=0}^{s-1} b_i \cdot k_i \quad (\text{A.4})$$

where:

$$k_i = f(x_n + c_i \cdot h, y_n + h \cdot \sum_{j=0}^{s-1} a_{i,j} \cdot k_j) \quad (\text{A.5})$$

satisfying:

$$\sum_{j=0}^{s-1} a_{i,j} = c_i \quad (\text{A.6})$$

A.2.2 Matricial notation (Butcher's)

Matricial notation is used to represent method's coefficients using a matrix.

For a s -stages **Runge-Kutta** method the matricial notation will be:

c_0	$a_{0,0}$	\cdots	$a_{0,s-1}$
\vdots	\vdots		\vdots
\vdots	\vdots		\vdots
c_{s-1}	$a_{s-1,0}$	\cdots	$a_{s-1,s-1}$
	b_0	\cdots	b_{s-1}



In section 10.2.1 is shown a data structure used to store the Butcher array.

A.3 Runge-Kutta types

There are several types of **Runge-Kutta** methods.

A.3.1 Implicit Runge-Kutta

A **Runge-Kutta** method is said to be implicit when the $a_{i,j} \neq 0$ for some $j > i$.

The 2-stages Gauss method is an implicit **Runge-Kutta** method of 2-stages:

$$\begin{array}{c|cc} \frac{3-\sqrt{3}}{6} & \frac{1}{4} & \frac{3-2*\sqrt{3}}{12} \\ \frac{3+\sqrt{3}}{6} & \frac{3+2*\sqrt{3}}{12} & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

A.3.2 Semi-implicit Runge-Kutta

A **Runge-Kutta** method is said to be semi-implicit when the $a_{i,j} = 0$ when $j > i$.

A 2-stages semi-implicit **Runge-Kutta** method:

$$\begin{array}{c|cc} \frac{3+\sqrt{3}}{6} & \frac{3+\sqrt{3}}{6} & 0 \\ \frac{3-\sqrt{3}}{6} & \frac{-\sqrt{3}}{3} & \frac{3+\sqrt{3}}{6} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

A.3.3 Explicit Runge-Kutta

A **Runge-Kutta** method is said to be explicit when the $a_{i,j} = 0$ when $j \geq i$.

A 4-stages explicit **Runge-Kutta** method also known as “**classic Runge-Kutta**”:

0		0			
$\frac{1}{2}$		$\frac{1}{2}$	0		
$\frac{1}{2}$		0	$\frac{1}{2}$	0	
$\frac{1}{2}$		0	0	1	0
1		0	0	1	0
<hr/>		$\frac{1}{6}$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{6}$

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